

# Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 03:10 am BST

PDB ID : 4HAZ

Title : Crystal structure of CRM1 inhibitor Leptomycin B in complex with CRM1(R

543S,K548E,K579Q)-Ran-RanBP1

Authors : Sun, Q.; Chook, Y.M.

Deposited on : 2012-09-27

Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.11

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

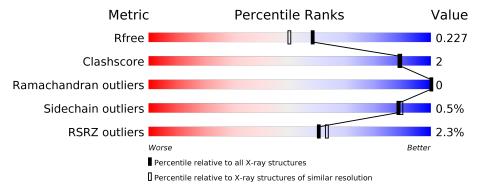
Validation Pipeline (wwPDB-VP) : 2.11

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar  resolution} \\ (\#{\rm Entries,  resolution  range(\AA)}) \end{array}$
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	A	216	89%	5% 6%
2	В	140	83%	• 14%
3	С	1023	94%	5% •



## 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12231 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called GTP-binding nuclear protein Ran.

$\mathbf{Mol}$	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	202	Total 1655	C 1067	N 284	O 298	S 6	0	4	0

• Molecule 2 is a protein called Ran-specific GTPase-activating protein 1.

Mo	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	121	Total 1005	C 636	N 176	O 189	S 4	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	98	LYS	ALA	CONFLICT	UNP P41920

• Molecule 3 is a protein called Exportin-1.

Mo	ol   Cl	hain	Residues	Atoms					ZeroOcc	${f AltConf}$	Trace
3		С	1014	Total 8319	C 5353	N 1353	O 1570	S 43	0	24	0

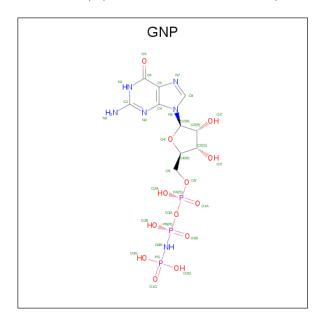
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	-1	GLY	_	EXPRESSION TAG	UNP P30822
С	0	ALA	_	EXPRESSION TAG	UNP P30822
С	539	CYS	THR	ENGINEERED MUTATION	UNP P30822
С	543	SER	ARG	ENGINEERED MUTATION	UNP P30822
С	548	GLU	LYS	ENGINEERED MUTATION	UNP P30822
С	579	GLN	LYS	ENGINEERED MUTATION	UNP P30822
С	1022	CYS	TYR	ENGINEERED MUTATION	UNP P30822

• Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter



code: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total 32	C 10	N 6	O 13	P 3	0	0

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

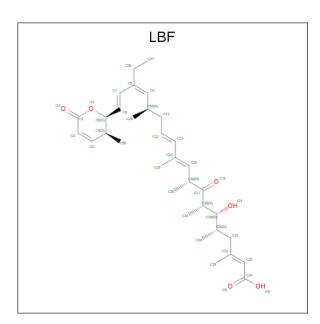
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0

• Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0
6	С	4	Total Cl 4 4	0	0

 $\bullet$  Molecule 7 is Leptomycin B (three-letter code: LBF) (formula:  $\mathrm{C_{33}H_{48}O_6}).$ 





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	С	1	Total 39	C 33	O 6	0	0

#### • Molecule 8 is water.

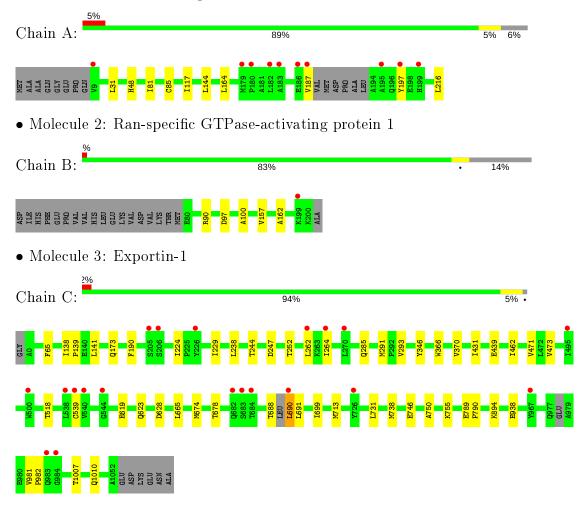
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	195	Total O 195 195	0	0
8	В	58	Total O 58 58	0	0
8	С	922	Total O 922 922	0	0



## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: GTP-binding nuclear protein Ran





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	105.82Å 105.82Å 305.23Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 - 1.90	Depositor
Resolution (A)	47.32 - 1.90	EDS
% Data completeness	99.8 (50.00-1.90)	Depositor
(in resolution range)	99.8 (47.32-1.90)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.58 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
P. P.	0.165 , $0.209$	Depositor
$R, R_{free}$	0.192 , $0.227$	DCC
$R_{free}$ test set	6882  reflections  (5.03%)	wwPDB-VP
Wilson B-factor $(\mathring{A}^2)$	27.1	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.33, 48.7	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12231	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, CL, MG, LBF

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond	lengths	Bond angles		
MIOI		RMSZ	# Z >5	RMSZ	# Z  > 5	
1	A	0.49	0/1701	0.56	0/2303	
2	В	0.44	0/1022	0.59	0/1363	
3	С	0.46	0/8533	0.52	0/11563	
All	All	0.47	0/11256	0.53	0/15229	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Α	1655	0	1652	7	0
2	В	1005	0	1005	4	0
3	С	8319	0	8420	33	0
4	A	32	0	13	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	С	4	0	0	0	0
7	С	39	0	46	1	0
8	A	195	0	0	0	0
8	В	58	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	С	922	0	0	3	0
All	All	12231	0	11136	41	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (41) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		$\operatorname{distance}\ ( ext{\AA})$	overlap (Å)
3:C:688:THR:HA	3:C:691:LEU:HD23	1.74	0.70
3:C:293[B]:VAL:HG12	3:C:346:TYR:CE2	2.36	0.61
2:B:97:ASP:O	2:B:100:ALA:O	2.21	0.58
3:C:244:THR:HG22	3:C:285:GLN:OE1	2.04	0.56
3:C:981:VAL:HG13	3:C:982:PRO:HD2	1.88	0.56
3:C:690:LEU:HB3	3:C:738:MET:HE1	1.88	0.55
3:C:1007:THR:H	3:C:1010:GLN:HE21	1.56	0.53
1:A:216:LEU:HD11	2:B:90:ARG:HG2	1.89	0.53
3:C:789[B]:GLU:HB2	3:C:790:PRO:HD3	1.92	0.51
3:C:238:LEU:O	3:C:252:THR:HG21	2.12	0.50
1:A:187:VAL:HG21	2:B:162:ALA:HB2	1.93	0.50
3:C:190:PHE:CZ	3:C:224:ILE:HG21	2.48	0.48
3:C:293[A]:VAL:HG23	8:C:1323:HOH:O	2.14	0.48
3:C:473:VAL:HG13	3:C:518:THR:HG22	1.95	0.47
3:C:229:ILE:HG13	3:C:262:LEU:HD11	1.96	0.47
3:C:173:GLN:NE2	8:C:1586:HOH:O	2.47	0.47
1:A:117:ILE:HB	1:A:144:LEU:HD22	1.97	0.47
1:A:81:ILE:HD11	3:C:65:PHE:CG	2.49	0.47
3:C:894:LYS:NZ	3:C:938:GLU:OE1	2.39	0.47
3:C:674:MET:O	3:C:678:THR:HG23	2.15	0.46
3:C:366:TRP:O	3:C:370:VAL:HG22	2.15	0.46
1:A:31:LEU:HD11	1:A:48[A]:HIS:CG	2.51	0.46
3:C:619:GLU:OE2	3:C:623:GLN:NE2	2.48	0.46
3:C:293[B]:VAL:HG12	3:C:346:TYR:CZ	2.49	0.46
3:C:439[A]:GLU:HB3	3:C:462[A]:ILE:HD11	1.99	0.45
7:C:1101:LBF:O5	7:C:1101:LBF:C33	2.65	0.44
3:C:789[A]:GLU:HB3	3:C:790:PRO:HD3	2.00	0.44
1:A:85:CYS:HB2	1:A:164:LEU:HD22	2.00	0.44
3:C:691:LEU:HD13	3:C:755:LYS:HZ3	1.82	0.43
3:C:264:ILE:HD11	8:C:1645:HOH:O	2.18	0.43
3:C:691:LEU:C	3:C:755:LYS:HZ1	2.22	0.43
3:C:138:ILE:HB	3:C:139:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({f \AA})$	overlap (Å)
3:C:665:LEU:HD13	3:C:713:MET:SD	2.58	0.42
1:A:187:VAL:CG2	2:B:162:ALA:HB2	2.49	0.42
3:C:431[B]:ILE:HD11	3:C:471:VAL:HG11	2.00	0.42
3:C:746:GLU:HB2	3:C:750:ALA:HB2	2.01	0.42
3:C:141:LEU:HD23	3:C:141:LEU:C	2.41	0.41
3:C:699:ILE:HG21	3:C:731:LEU:HD21	2.02	0.41
3:C:247:ASP:N	3:C:247:ASP:OD2	2.54	0.40
3:C:439[A]:GLU:HB3	3:C:462[A]:ILE:CD1	2.51	0.40
3:C:238:LEU:HD22	3:C:252:THR:HG23	2.04	0.40

There are no symmetry-related clashes.

#### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	$_{ m ntiles}$
1	A	$202/216 \ (94\%)$	198 (98%)	4 (2%)	0	100	100
2	В	120/140 (86%)	113 (94%)	7 (6%)	0	100	100
3	С	1032/1023 (101%)	1015 (98%)	17 (2%)	0	100	100
All	All	1354/1379 (98%)	1326 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	179/185~(97%)	178 (99%)	1 (1%)	86 87
2	В	105/122~(86%)	104 (99%)	1 (1%)	76 76
3	С	$950/933 \; (102\%)$	946 (100%)	4 (0%)	91 91
All	All	1234/1240 (100%)	1228 (100%)	6 (0%)	88 89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	TYR
2	В	157	VAL
3	С	291	MET
3	С	539	CYS
3	С	628	ASP
3	С	690	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	205	GLN
3	С	35	GLN
3	С	434	ASN
3	С	1010	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.



## 5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Mol Type Chain Res		Res Link		Bond lengths		Bond angles				
MIOI	туре	Chain	nes	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GNP	A	301	5	28,34,34	2.67	7 (25%)	30,54,54	1.43	3 (10%)	
7	LBF	С	1101	3	35,39,39	2.30	4 (11%)	35,52,52	2.77	9 (25%)	

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

$\mathbf{Mol}$	$\mathbf{Type}$	Chain	${f Res}$	Link	Chirals	Torsions	Rings
4	GNP	A	301	5	-	3/17/38/38	0/3/3/3
7	LBF	С	1101	3	-	1/43/58/58	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$Ideal(\AA)$
4	A	301	GNP	C4-N9	-11.38	1.32	1.47
7	С	1101	LBF	C2-C3	10.14	1.53	1.33
7	С	1101	LBF	O2-C1	6.98	1.46	1.35
4	A	301	GNP	PG-N3B	3.88	1.73	1.63
4	A	301	GNP	PB-N3B	3.78	1.73	1.63
7	С	1101	LBF	C2-C1	3.03	1.51	1.44
4	A	301	GNP	C8-N9	-2.99	1.35	1.45
4	A	301	GNP	C5-C6	-2.74	1.48	1.52
7	С	1101	LBF	O2-C5	-2.44	1.43	1.46
4	A	301	GNP	C2-N1	-2.30	1.34	1.44
4	A	301	GNP	PB-O3A	2.14	1.61	1.59

All (12) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
7	С	1101	LBF	C3-C2-C1	-8.84	114.02	121.40
7	С	1101	LBF	C4-C3-C2	-8.35	114.64	123.50
7	С	1101	LBF	O2-C1-C2	6.56	122.72	117.98
4	A	301	GNP	O1G-PG-N3B	-5.00	104.40	111.77
7	С	1101	LBF	C26-C8-C9	-4.77	119.95	126.39
4	A	301	GNP	C4-C5-N7	3.48	107.07	102.46
7	С	1101	LBF	O1-C1-C2	-3.42	119.64	126.00
7	С	1101	LBF	C11-C12-C13	-3.25	118.74	126.00
4	A	301	GNP	PA-O3A-PB	-2.47	123.91	132.62
7	С	1101	LBF	C29-C14-C13	2.18	121.51	118.08
7	С	1101	LBF	C5-C6-C7	-2.06	120.61	124.94
7	С	1101	LBF	C10-C9-C8	-2.05	124.57	128.25

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GNP	PG-N3B-PB-O1B
4	A	301	GNP	C2'-C1'-N9-C4
7	С	1101	LBF	C27-C26-C8-C9
4	A	301	GNP	PG-N3B-PB-O3A

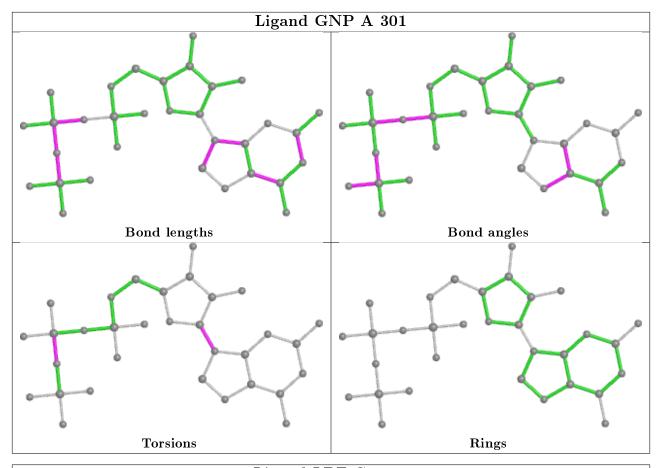
There are no ring outliers.

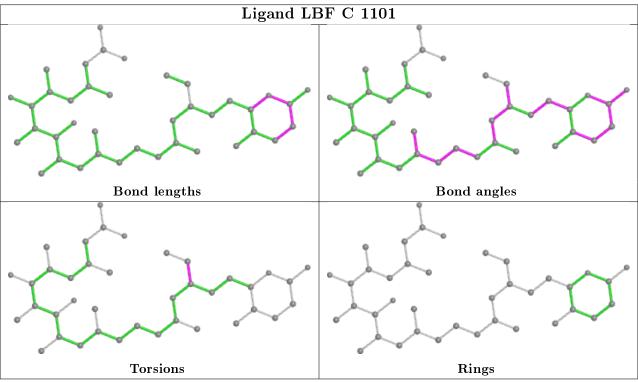
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	С	1101	LBF	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

#### 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	202/216~(93%)	0.01	10 (4%) 28 32	14, 20, 43, 61	0
2	В	121/140 (86%)	-0.16	1 (0%) 86 87	21, 30, 48, 74	0
3	С	1014/1023 (99%)	-0.13	20 (1%) 65 68	13, 24, 48, 84	0
All	All	1337/1379 (96%)	-0.11	31 (2%) 60 63	13, 24, 48, 84	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	С	264	ILE	5.2
1	A	195	ALA	4.5
3	С	205	SER	4.3
1	A	182	LEU	3.6
3	С	226	TYR	3.6
3	С	262	LEU	3.5
3	С	206	SER	3.5
3	С	983	GLN	3.4
3	С	540	VAL	3.3
3	С	683	SER	3.3
2	В	199	LYS	3.1
1	A	197	TYR	3.1
3	С	684	THR	3.0
1	A	9	VAL	2.9
1	A	179	MET	2.8
3	С	690	LEU	2.4
1	A	180	PRO	2.4
3	С	984	GLY	2.4
1	A	187	VAL	2.4
1	A	199	HIS	2.3
3	С	726	TYR	2.3
1	A	186	GLU	2.3
3	С	544	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	С	500	TRP	2.2
3	С	967	TYR	2.2
3	С	270	LEU	2.2
3	С	538	LEU	2.2
1	A	183	ALA	2.2
3	С	682	GLN	2.1
3	С	539	CYS	2.1
3	С	495	ILE	2.0

#### 6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

#### 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

### 6.4 Ligands (i)

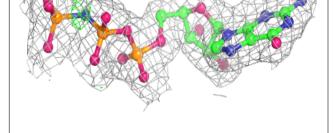
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

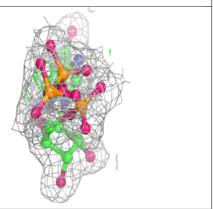
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}({ ext{\AA}}^2)$	Q < 0.9
6	CL	С	1105	1/1	0.86	0.05	77,77,77,77	0
6	CL	A	303	1/1	0.92	0.32	72,72,72,72	0
6	CL	С	1102	1/1	0.93	0.18	70,70,70,70	0
7	LBF	С	1101	39/39	0.94	0.18	23,33,44,47	0
6	CL	С	1104	1/1	0.97	0.12	65,65,65,65	0
6	CL	С	1103	1/1	0.97	0.22	51,51,51,51	0
5	MG	A	302	1/1	0.98	0.06	13,13,13,13	0
4	GNP	A	301	32/32	0.99	0.09	16,18,20,21	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



# Electron density around LBF C 1101: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $mF_o$ -DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive) Electron density around GNP A 301: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $mF_o$ -DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive)







## 6.5 Other polymers (i)

There are no such residues in this entry.

